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Our previous semiempirical treatments have been based on the ZDO approximations introduced by Pople, MNDO and AMI using the best of these (NDDO). Although there were good reasons to believe that the ZDO approximation is wholly unacceptable, we were forced to use it in order to obtain a treatment of practical value, i.e. one that could be applied directly to the molecules of interest to organic chemists rather than to meaninglessly simplified "models", using generally available computers. Although the resulting treatments proved remarkably successful and have led to major developments in chemical theory, in particular in studies of reaction mechanisms. The situation has, however, changed dramatically in recent years with the almost incredible increase in computing power of minicomputers, due to the invention of the integrated circuit. The primary purpose of the research supported by this grant was to make use of the greatly improved computing facilities now available to us to develop a semiempirical treatment based on a full LCAC SLF MO approximation, i.e. one in which overlap is retained.

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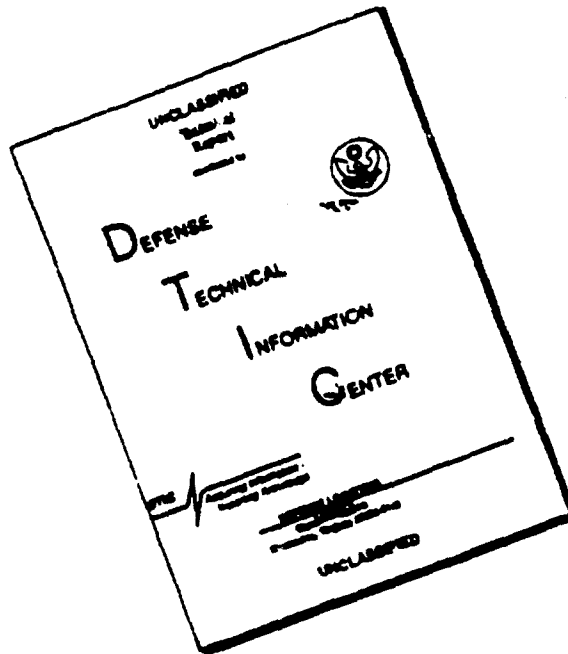
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FINAL REPORT AFOSR F49620-92-J-0107 Michael J.S. Dewar

Technical Report Grant #166636212

Our previous semiempirical treatments have been based on the ZDO approximations introduced by Pople, MNDO and AM1 using the best of these (NDDO). Although there were good reasons to believe that the ZDO approximation is wholly unacceptable, we were forced to use it in order to obtain a treatment of practical value, i.e. one that could be applied directly to the molecules of interest to organic chemists rather than to meaninglessly simplified "models", using generally available computers. Although the resulting treatments proved remarkably successful and have led to major developments in chemical theory, in particular in studies of reaction mechanisms, the situation has, however, changed dramatically in recent years with the almost incredible increase in computing power of minicomputers, due to the invention of the integrated circuit. The primary purpose of the research supported by this Grant was to make use of the greatly improved computing facilities now available to us to develop a semiempirical treatment based on a full LCAO SCF MO approximation, i.e. one in which overlap is retained.

This at one stroke has completely revolutionized the semiempirical approach because there are now no restrictions on the type of ab initio treatment that can be parametrized. Since parametrization is bound to increase the accuracy of any ab initio treatment while simultaneously reducing the computing time needed, there can now be no question that this is the approach to follow if one is concerned with practical applications of quantum theory to chemical problems. The situation clearly needs to be recognized by an appropriate change in nomenclature. We have therefore termed this approach the *Semi-Ab-Initio* (SA) method, our first treatment of the kind being *Semi-Ab-Initio Model 1* (SAM1).

SAM1 is based on Pople's STO-3G approximation with one further simplification. Since there seem to be no strong specific objections to the core approximation, we have made it to save computing time. We have written a computer program for SAM1 and parametrized it for the "organic" elements (C,H,N,O) and the halogens (F,Cl,Br,I). Calculations for a large number of molecules and positive and negative ions, and for a number of chemical reactions, have shown it to be clearly superior to our previous semiempirical procedures (MNDO, AM1) and to Stewart's PM3 procedure, a somewhat dubious reparametrization of AM1. The extra computing time needed is also quite small, less than an order of magnitude. This work was reported in a recent paper in *Tetrahedron* [1] and a further publication has appeared in *Accounts of Chemical Research* [2], reviewing contributions to the theory of reaction mechanisms due to calculations carried out with support from AFOSR.

I have now retired completely from chemistry. The work on SAM1 is being officially continued by Dr. Andrew J. Holder at the University of Missouri in Kansas City.

In conclusion I would like once again, and for the last time, to acknowledge the far sighted support I have had for many years from AFOSR. Without it I could not have carried out the work I have done in theoretical chemistry.

[1] M. J. S. Dewar, C. Jle, and J. Yu, *Tetrahedron* 49, 5003-5008 (1993).

[2] M. J. S. Dewar and C. Jle, *Acc. Chem. Res.* 25, 537-543 (1992).

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